Supplementary Information for

Adsorption and capacitive regeneration of nitrate using inverted capacitive deionization with surfactant functionalized carbon electrodes

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Abstract

This document contains supplementary information and figures demonstrating (1) nitrate affinity (vs. chloride ions) of cetrimonium bromide (CTAB), and (2) adsorption performance of a CDI cell with CTAB-treated active electrode and untreated counter electrode.

S-1. Nitrate affinity of CTAB-treated carbon electrode

As mentioned in the main text, resins functionalized with trimethyl quaternary amine groups show affinity toward nitrate ions.[1,2] Additionally, CTAB (a quaternary ammonium surfactant) is known to adsorb onto activated carbon surface, and in turn, passively (in the absence of voltage) adsorb ions such as perchlorate.[3–5] We here demonstrate preferential adsorption of selected anions to CTAB-treated carbon electrode. To this end, we fabricated an i-CDI cell with CTAB-treated and SDBS-treated electrodes, each with dry mass of 0.41 g. We operated this i-CDI cell at 1 V for 5 h (regeneration step) followed by 0 V for another 5 h (adsorption step) under 0.73 ml min^{-1} constant flowrate. Feed solution was 2 mM NaCl and 2 mM $NaNO_3$. Effluent solution was collected over 15 min intervals into separate containers, and concentration of chloride and nitrate ions was measured by ion chromatography (DIONEX DX 500, DIONEX, CA, USA) at Stanford ICP-MS/TIMS Facility. Figure S1 shows chloride and nitrate adsorption capacity of our i-CDI cell over adsorption step (in units of moles of anion adsorbed per gram of CTAB-treated electrode). Results show about 25 and 120 µmol g^{-1} (equivalent to 0.9 and 7.4 mg g^{-1}) adsorption capacity for chloride and nitrate ions, respectively. Figure S1 thus clearly shows nitrate affinity of CTAB-treated electrode.

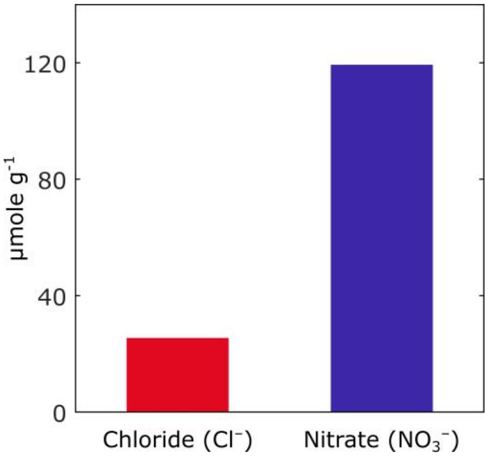

Figure S1. Preferential nitrate adsorption to an i-CDI cell with CTAB-treated and SDBS-treated electrodes. We operated the cell at 1 V regeneration and 0 V adsorption steps for 5 h each. Results show chloride and nitrate adsorption capacity of i-CDI cell in units of moles of anion per mass of CATB-treated electrode.

S-2. CDI cell with CTAB-treated active electrode and untreated counter electrode

In addition to i-CDI cell presented in the main text, we also built a cell consisting of one CTAB-treated electrode (as active electrode) and one untreated porous carbon electrode (as the counter electrode). Cell geometry and electrodes mass were approximately the same as those of the i-CDI cell in the main text. Figure S2 shows measured effluent concentration and electric current upon application of 0.8 V and 0 V external voltages. Interestingly, results show negligible salt adsorption for this comparison case versus to the results in Figure 2 of the main text. We observe this negligible adsorption despite the fact that the magnitude of electric current is comparable to that of our i-CDI cell with CTAB-treated and DBS-treated electrodes. We attribute this negligible salt adsorption to simultaneous expulsion and adsorption of

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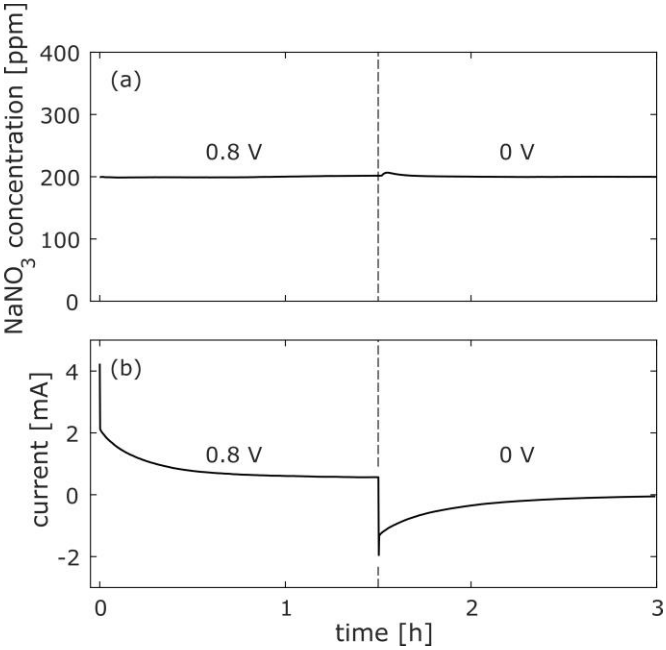

Figure S2. Measured (a) effluent salt concentration and (b) electric current for the CDI cell made with CTAB-treated active electrode and untreated counter electrode at 0.8 V and 0 V external voltages. We hypothesize negligible salt adsorption is due to simultaneous expulsion and adsorption of nitrate ions from the electrodes. See Figure 2 of the main text for more information.

nitrate ions from the electrodes. For example, when 0.8 V is applied to the cell, nitrate is expelled from CTA-AC active electrode and is simultaneously electrostatically adsorbed to the untreated, porous counter electrode. The reverse occurs for 0 V applied (short circuit between electrodes). This behavior is in contrast to our i-CDI cell with both CTA-AC and DBS-AC electrodes. For the latter cell, the negatively charged surfactant ion on the DBS-AC electrode surface likely electrostatically shields nitrate from re-adsorption to the electrode. This comparison experiment here is presented here to highlight the importance of treating both electrodes of the i-CDI cell.

References

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